

\mathbb{Z}_2 Green's function topology of Majorana wires

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We calculate the \mathbb{Z}_2 topological invariant characterizing a one dimensional topological superconductor using a Wess-Zumino-Witten dimensional extension. The invariant is formulated in terms of the single particle Green's function which allows to classify interacting systems. Employing a recently proposed generalized Berry curvature method, the topological invariant is represented independent of the extra dimension requiring only the single particle Green's function at zero frequency of the interacting system. Furthermore, a modified twisted boundary conditions approach is used to rigorously formulate the topological invariant for disordered systems.

Introduction. The key feature of a topological superconductor (TSC) in one spatial dimension (1D) [1–4] is a holographic single Majorana bound state (MBS) associated with each of its ends which is topologically protected by particle hole symmetry (PHS). The recently proposed realization of the 1D TSC in an InSb nanowire with strong spin orbit interaction (SOI) and proximity induced s-wave superconductivity [2, 3] is so far the most promising candidate as to its experimental feasibility. Very recently, first experimental signatures of MBS have been reported by several experimental groups [5–7], however, it should be mentioned that alternative explanations for robust zero bias resonances not owing to Majorana zeromodes have been brought forward [8, 9]. Note that PHS in this class of systems does not imply a true limitation on the band structure of the normal-conducting spin orbit coupled quantum wire but is emergent from the Bogoliubov-deGennes (BdG) mean field description of superconductivity. An additional chiral symmetry present in the ideal model systems proposed in Refs. [2, 3] promotes the \mathbb{Z}_2 invariant characterizing the presence of an unpaired MBS to a \mathbb{Z} invariant [10, 11] counting the number of zeromodes at each edge. However, perturbations modifying the SOI as well as magnetic impurities can break the chiral symmetry and gap out paired MBS. The influence of interactions on the topological classification of chiral 1D systems has been analyzed from a matrix product state perspective [12]. Very recently, the classification of a chiral 1D system in terms of its single particle Green's function has been reported [13]. The robustness of the TSC phase in interacting nanowires has been investigated using renormalization group (RG) methods [14–16].

In this work, we go beyond the \mathbb{Z}_2 classification in terms of the Pfaffian of the Hamiltonian in Majorana representation reported in Ref. [1] by including disorder and adiabatic interactions into the classification scheme. We present the \mathbb{Z}_2 -classification of the 1D TSC phase which, without additional symmetries, generically belongs to the Cartan-Altland-Zirnbauer class D [17],

in terms of its single particle Green's function. In a first step, we work out explicitly a dimensional extension procedure for a realization of the 1D TSC in a nanowire with strong SOI and proximity induced s-wave superconductivity [2, 3]. This allows us to reduce the topological classification of the 1D TSC to the quantum anomalous Hall (QAH) effect [18] of the extended 2D system. This procedure fits into the general classification framework of topological field theory (TFT) proposed for time reversal invariant topological insulators in Refs. [19, 20] and allows for a reformulation of the invariant in terms of the single particle Green's function. Upon switching on interactions adiabatically, our classification remains valid for Luttinger liquid like interactions as argued in Ref. [21]. Thereafter, we employ a recently proposed generalized Berry curvature method [22] showing that the interacting invariant can be expressed in terms of the zero frequency single particle Green's function of the physical 1D system, which is independent of the previously introduced extra dimension. Finally, we demonstrate how a hybrid approach of twisted boundary conditions (TBC) [23] in the physical dimension and periodic boundary conditions in the extra dimension can be used to additionally include disorder at the level of the bulk topological invariant, i.e. without probing the presence of unpaired MBS, quantized zero bias resonances, or other finite size effects.

Model of the 1D TSC. A lattice model of the 1D TSC [2, 11] can be cast into the form $H = \int \Psi^\dagger \mathcal{H}_{BdG} \Psi$, where the basis is chosen such that $\Psi = (\psi_\uparrow, \psi_\downarrow, \psi_\uparrow^\dagger, \psi_\downarrow^\dagger)$. In this basis

$$\mathcal{H}_{BdG} = \begin{pmatrix} H_0 & \delta \\ \delta^\dagger & -H_0^* \end{pmatrix}.$$

For the 1D TSC, $H_0(k) = \xi_k + B\sigma_x + u \sin(k)\sigma_y$ is the Hamiltonian of a single channel quantum wire in the presence of a B -field induced Zeeman splitting and Rashba SOI. The proximity induced s-wave superconducting gap is of the form $\delta = \begin{pmatrix} 0 & -\Delta \\ \Delta & 0 \end{pmatrix}$ and $\xi_k = 1 - \cos k - \mu$. Introducing the set of Pauli-matrices τ_i for the particle

hole pseudo spin, the BdG Bloch Hamiltonian reads

$$H_{\text{BdG}}(k) = (\xi_k + B\sigma_x + u \sin(k)\sigma_y)\tau_z + \Delta\sigma_y\tau_y. \quad (1)$$

In this representation, the PHS operation has the intuitive form

$$C = \tau_x K, \quad (2)$$

where K denotes complex conjugation. Let us very briefly review the salient physics starting from the continuum model obtained from Eq. (1) by substituting $\sin(k) \rightarrow k$, $\cos(k) \mapsto 1 - \frac{k^2}{2}$. For $B = \Delta = 0 \neq u$, the band structure consists of two particle hole symmetric copies (emergent from the BdG picture) of the shifted Rashba parabulae. The lattice regularization in Eq. (1) is introduced to make the topological invariants well defined. $\Delta \neq 0$ gaps out the system in its entire Brillouin zone (BZ). For small k this gap competes with a Zeeman gap due to $B \neq 0$ leading to a band inversion at $B^2 = \mu^2 + \Delta^2$. For $B^2 > \mu^2 + \Delta^2$ we have a TSC with a single MBS associated with each end of a finite wire.

Dimensional extension. Following the general outline in Ref. [19], we explicitly perform a dimensional extension introducing an extra coordinate v , thus reducing the topological classification of the noninteracting model to the analysis of the QAH effect of the extended 2D system. The idea is quite simple: Our system cannot be deformed into a trivial 1D insulator without breaking PHS which provides the topological protection of the TSC phase. However, breaking this symmetry we can deform the TSC, say upon varying v from 0 to π , into a trivial 1D superconductor without ever closing the bulk gap of the instantaneous system. If we were to investigate the QAH features, i.e. the first Chern number \mathcal{C} , of the 2D system resulting from such an interpolation, the integer would totally depend on our choice of the interpolation. However, performing the interpolation also for $v \in [-\pi, 0]$ in such a way that the resulting 2D system is 2π -periodic in v , PHS preserving, and insulating, \mathcal{C} is well defined up to even integers.

This means that a \mathbb{Z}_2 information $\nu = \mathcal{C}(\text{mod } 2)$ is well defined and only depends on the physical 1D system. It is worth noting that finding a suitable interpolation is non-trivial and requires some insight into the physical mechanisms underlying the model. In the following, we will explicitly present an extension which works for a generic 1D TSC and can also be used later on for the disordered interacting system. The guiding physical idea is as follows: Switch on a particle hole breaking gap $\sim \sin(v)\tau_x$ which will keep the gap open for $v \neq 0, \pi \pmod{2\pi}$. Destroy the band inversion by a term $\sim \beta(2 - 2\cos v)\sigma_y\tau_y$ which vanishes for the physical model ($v = 0$) and will for sufficiently large β produce a trivial superconducting phase for $v = \pm\pi$ where it enhances the superconducting gap by 4β . In summary, the Wess-Zumino-Witten (WZW)

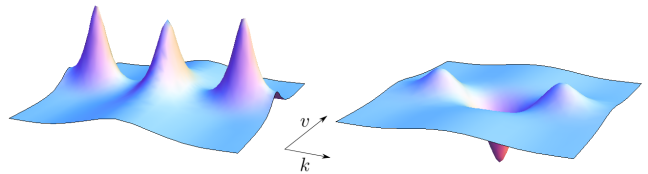


FIG. 1. (Color online) 3D plot of the Berry curvature $\mathcal{F}(k, v)$ for nontrivial parameters ($B = 1.5$) left and trivial parameters ($B = 0.4$) right. $u = \Delta = 2\beta = 1$, $\mu = 0$ in both plots.

[24] extended Hamiltonian reads

$$\mathcal{H}_{\text{WZW}}(k, v) = H_{\text{BdG}}(k) + \sin(v)\tau_x + \beta(2 - 2\cos v)\sigma_y\tau_y. \quad (3)$$

Integrating the Berry curvature \mathcal{F} of this Hamiltonian over the (k, v) BZ indeed yields

$$\mathcal{C} = \frac{1}{2\pi} \int_{\text{BZ}} \mathcal{F} = \theta(B^2 - \Delta^2 - \mu^2), \quad (4)$$

valid for parameters close enough to the band inversion that no artificial level crossings which depend on the details of the lattice regularization occur.

In Fig. 1, we compare the Berry curvature of an extension of a nontrivial 1D TSC with that of a trivial superconducting wire. In the extra dimension v , the modulus of the curvature is smoothly decaying without any notable difference between the trivial and the nontrivial case. This is reflected in our derivation below, which shows that the topological invariant of the translation-invariant system can be defined in terms of its single particle Green's function without reference to the extra dimension. Note that this picture changes in the framework of TBC as introduced to account for the presence of disorder as is discussed below and shown in Fig. 2.

Single particle Green's function topology. We now discuss the possibility to include interactions into the proposed classification scheme by generalizing the Chern number of the noninteracting system to a topological invariant of the single particle Green's function in combined frequency momentum space, as has been proposed for time reversal invariant topological insulators in 2D and 3D [20]. In even spatial dimension $2n$, it has been shown [25–27] that the homotopy of the single particle Green's function determines the Hall conductivity σ_{xy} ($n = 1$) and its higher dimensional analogues, respectively, of an insulating fermionic system. It has been explicitly demonstrated [19] that this representation of σ_{xy} adiabatically connects to the n th-Chern number associated with the Berry curvature of a Bloch Hamiltonian in the non-interacting limit. The adiabatic assumption in this case implies that the gapped ground state of the

interacting system can be continuously connected to the manifold of occupied single particle levels of the noninteracting system which is also separated from the empty states by a finite energy gap. The most prominent example of interactions which are non-adiabatic in the sense just defined lead to the $\frac{1}{\nu}$ fractional quantum Hall (FQH) effect in a partially filled lowest Landau level (LLL). In this case, the noninteracting system is gapless and the single particle states that span the LLL split into ν degenerate ground states when TBC are applied [23]. This ground state degeneracy is at the basis of the concept of topological order [28] which rigorously classifies FQH systems.

In 1D, interactions play a peculiar role generically leading to non-Fermi-liquid behavior. From a viewpoint of perturbation theory interactions are therefore considered to be non-adiabatic in 1D, as no meaningful quasiparticles can be defined. However, it has been argued [21] that the Fermi surface properties as described by the momentum space topology of the single particle Green's function are still adiabatically connected to those of the non-interacting system.

Rewritten in terms of the single particle Green's function $G(\omega, p)$ of the extended system, i.e. $G_0(\omega, p) = (i\omega - \mathcal{H}_{\text{WZW}}(p))^{-1}$ for the special case of the non-interacting system, the \mathbb{Z}_2 invariant ν reads

$$\nu = \frac{\epsilon^{\mu\nu\rho}}{24\pi^2} \int_{BZ \times \mathbb{R}_\omega} \text{Tr} [GG_\mu^{-1}GG_\nu^{-1}GG_\rho^{-1}] \pmod{2}, \quad (5)$$

where $G_\mu^{-1} = \partial_\mu G^{-1}$, $\mu = 0, 1, 2 = \omega, k, v$. Very recently, it has been generally shown [22] that for an interacting system, an invariant of this form can be simplified by introducing a generalized Berry curvature $\tilde{\mathcal{F}} = -i \sum_{R\text{-zeros}} (d\langle p, \alpha |) \wedge d|p, \alpha \rangle$ associated with the fictitious non-interacting Hamiltonian $\tilde{H} = -G^{-1}(0, p)$, which takes into account the eigenvectors $|p, \alpha \rangle$ of $G^{-1}(0, p)$ with positive eigenvalues, the so called R-zeros [22]. The \mathbb{Z}_2 invariant then takes the form of a generalized Chern number, i.e.

$$\nu = \frac{1}{2\pi} \int_{BZ} \tilde{\mathcal{F}} \pmod{2}. \quad (6)$$

As has been shown for the noninteracting case in Ref. [19] the \mathbb{Z}_2 classification of the particle hole symmetric 1D system can then be further simplified to

$$\nu = 2P(0) \pmod{2} = \frac{1}{\pi} \int_0^{2\pi} dk \tilde{\mathcal{A}}(k) \pmod{2}, \quad (7)$$

where $P(0)$ is the charge polarization of the physical 1D system and $\tilde{\mathcal{A}}(k) = -i \sum_{R\text{-zeros}} \langle k, \alpha | d|k, \alpha \rangle$ is the generalized Berry connection restricted to the physical system at $v = 0$, i.e. at $p = (k, 0)$. Note that this general form does no longer depend on the dimensional extension procedure and can be calculated once the

zero frequency single particle Green's function $G(0, k)$ is known. Finally, the \mathbb{Z}_2 -invariant can be practically calculated by formal analogy to the non-interacting case by calculating the Majorana number [1] defined in terms of the Pfaffian of the fictitious non-interacting Hamiltonian \tilde{H} in Majorana representation.

Disorder and Twisted Boundary Conditions. Our formulation so far has been relying on translation-invariance which implies the existence of a BZ. This description will thus no longer be applicable in the presence of disorder. To this end, the concept of TBC has been introduced to topologically classify quantum Hall systems in the absence of translation-invariance [23]. As long as a bulk mobility gap is present, the Green's function is exponentially bounded in real space for energies in this gap. Under these conditions, Niu *et al.* [23] show that the Hall conductivity can be represented as a constant ground state Berry curvature with the wave vector replaced by the twisting angles θ, ϕ of the TBC. In this formalism, the Hall conductivity σ_{xy} reads

$$\begin{aligned} \sigma_{xy} &= 2\pi i G_0 \left(\langle \frac{\partial \psi_0}{\partial \theta} | \frac{\partial \psi_0}{\partial \phi} \rangle - \langle \frac{\partial \psi_0}{\partial \phi} | \frac{\partial \psi_0}{\partial \theta} \rangle \right) \equiv \\ &2\pi i G_0 \mathcal{F}_{\theta\phi} = G_0 \int_{T^2} \frac{i\mathcal{F}_{\theta\phi}}{2\pi}, \end{aligned} \quad (8)$$

where ψ_0 denotes the ground state wave function, $G_0 = \frac{e^2}{h} = \frac{1}{2\pi}$ is the quantum of conductance. In last equality of Eq. (8), the independence of $\mathcal{F}_{\theta\phi}$ on the twisting angles [23] has been used to make the topological quantization of σ_{xy} manifest by representing it as G_0 times the Chern number of the $U(1)$ -bundle over the torus T^2 of the twisting angles (θ, ϕ) . Since in this work, we consider a disordered 1D system, we can without loss of generality assume translation-invariance in the extra dimension. Integrating over the momentum v associated with the direction of translational invariance is equivalent to evaluating Eq. (8) for $\theta = 0$ for the special case of a system with translational invariance in x -direction. Within this hybrid approach of twisted boundary conditions in the physical dimension and v -momentum integration in the extra dimension, the Chern number of the extended 2D system in the presence of this stripe-like disorder can be expressed as

$$\mathcal{C} = \int_{-\pi}^{\pi} dv \int_{-\pi}^{\pi} d\phi \frac{\hat{\mathcal{F}}_{v\phi}}{2\pi} = \int_{-\pi}^{\pi} dv \hat{\mathcal{F}}_{v\phi} \quad (9)$$

where $\hat{\mathcal{F}}$ is the Berry curvature on the "mixed" torus defined by the wave vector in v -direction and the twisting angle ϕ of the TBC imposed in the physical direction. The first equality sign in Eq. (9) makes the integer quantization of our topological invariant manifest, whereas the second equality sign follows from the independence of $\int_0^{2\pi} dv \hat{\mathcal{F}}_{v\phi} = \mathcal{F}_{\theta\phi}|_{\theta=0}$ of the twisting angle ϕ . The

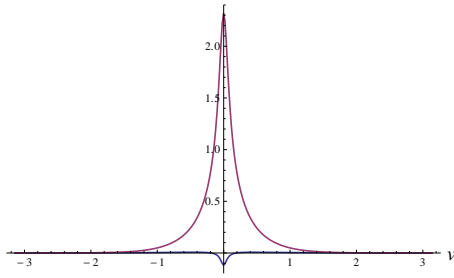


FIG. 2. (Color online) Plot of the Berry curvature $\hat{\mathcal{F}}_{v,\phi}|_{\phi=0}$, for nontrivial parameters ($\Delta = 0.7$, $\gamma = u = B = \beta = 1$, $\mu = 0$) (purple) and trivial parameters ($\Delta = 0.7$, $\gamma = 5$, $u = B = \beta = 1$, $\mu = 0$) (blue). Wire length 100 sites in both plots.

main advantage of Eq. (9) as compared to the general 2D case (see Eq. (8)) is that only the eigenstates of a 1D system have to be calculated to evaluate the topological invariant which is numerically less costly. This program allows for a topological classification of disordered systems with periodic boundaries, i.e. without explicitly probing the presence of unpaired MBS. The influence of disorder on the presence of MBS has been studied using a scattering matrix approach [29, 30].

In Fig. 2, we show the mixed Berry curvature $\hat{\mathcal{F}}_{v,\phi}|_{\phi=0}$ for a weakly disordered system ($\gamma = 1$) in the topologically nontrivial phase and a strongly disordered trivial system ($\gamma = 5$). Here, γ is the strength of a scalar Gaussian onsite potential. Note that in contrast to the translation-invariant case (see Eq. (7)) the topology is determined by the v -dependence of the mixed Berry curvature. Finally, we would like to point out that even for $\gamma = 1$, the onsite potential fluctuations significantly exceed the bulk insulating gap of the 1D TSC. The disorder-induced transition from nontrivial to trivial takes place at disorder strengths which are, depending on the other model parameters typically three to five times larger than the bulk gap which is in agreement with recent results obtained from level spectroscopy in 1D TSC with closed boundary conditions [31].

Conclusions. We have constructed a dimensional extension which reduces the topological classification of the 1D TSC phase to the QAH effect in two dimensions. This approach is ready-made to rephrase the invariant in terms of the single particle Green's function of the extended system. Using a generalized Berry curvature method, the invariant can be simplified to the noninteracting classification scheme with a fictitious non-interacting Hamiltonian defined in terms of the Green's function of the physical 1D system at zero frequency. To obtain a well defined topological invariant for disordered systems, the method of TBC has been modified to a hybrid approach accounting for the partial

translation invariance in the extra dimension.

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- [1] A. Kitaev, Physics-Uspekhi **44**, 131 (2001).
 - [2] R. M. Lutchyn, J. D. Sau, and S. Das Sarma, Phys. Rev. Lett. **105**, 077001 (2010).
 - [3] Y. Oreg, G. Refael, and F. von Oppen, Phys. Rev. Lett. **105**, 177002 (2010).
 - [4] C. W. J. Beenakker, arXiv:1112.1950 (2011).
 - [5] V. Mourik, K. Zuo, S. M. Frolov, S. R. Plissard, E. P. A. M. Bakkers, and L. P. Kouwenhoven, Science **336**, 1003 (2012).
 - [6] M. T. Deng, C. L. Yu, G. Y. Huang, M. Larsson, P. Caroff, and H. Q. Xu, arXiv:1204.4130 (2012).
 - [7] A. Das, Y. Ronen, Y. Most, Y. Oreg, M. Heiblum, and H. Shtrikman, arXiv:1205.7073 (2012).
 - [8] D. Bagrets and A. Altland, arXiv:1206.0434 (2012).
 - [9] J. Liu, A. C. Potter, K. T. Law, and P. A. Lee, arXiv:1206.1276 (2012).
 - [10] S. Ryu and Y. Hatsugai, Phys. Rev. Lett. **89**, 077002 (2002).
 - [11] S. Tewari and J. D. Sau, arXiv:1111.6592 (2011).
 - [12] L. Fidkowski and A. Kitaev, Phys. Rev. B **83**, 075103 (2011).
 - [13] S. R. Manmana, A. M. Essin, R. M. Noack, and V. Gurarie, arXiv:1205.5095 (2012).
 - [14] S. Gangadharaiah, B. Braunecker, P. Simon, and D. Loss, Phys. Rev. Lett. **107**, 036801 (2011).
 - [15] E. Sela, A. Altland, and A. Rosch, Phys. Rev. B **84**, 085114 (2011).
 - [16] A. M. Lobos, R. M. Lutchyn, and S. Das Sarma, arXiv:1202.2837 (2012).
 - [17] A. Altland and M. R. Zirnbauer, Phys. Rev. B **55**, 1142 (1997).
 - [18] F. D. M. Haldane, Phys. Rev. Lett. **61**, 2015 (1988).
 - [19] X.-L. Qi, T. L. Hughes, and S.-C. Zhang, Phys. Rev. B **78**, 195424 (2008).
 - [20] Z. Wang, X.-L. Qi, and S.-C. Zhang, Physical Review Letters **105**, 256803 (2010).
 - [21] G. E. Volovik, *The Universe in a Helium Droplet* (Clarendon Press, 2003).
 - [22] Z. Wang and S.-C. Zhang, arXiv:1203.1028 (2012).
 - [23] Q. Niu, D. J. Thouless, and Y.-S. Wu, Phys. Rev. B **31**, 3372 (1985).
 - [24] E. Witten, Nuclear Physics B **223**, 422 (1983).
 - [25] A. N. Redlich, Phys. Rev. D **29**, 2366 (1984).
 - [26] G. Volovik, JETP **67(9)**, 1804 (1988).
 - [27] M. F. L. Golterman, K. Jansen, and D. B. Kaplan, Physics Lett. B **301**, 219 (1993).
 - [28] X.-G. Wen, Int. J. Mod. Phys. B **4**, 239 (1990).
 - [29] P. W. Brouwer, M. Duckheim, A. Romito, and F. von Oppen, Phys. Rev. Lett. **107**, 196804 (2011).
 - [30] P. W. Brouwer, M. Duckheim, A. Romito, and F. von Oppen, Phys. Rev. B **84**, 144526 (2011).
 - [31] A. M. Cook, M. M. Vazifeh, and M. Franz, arXiv:1206.3829 (2012).